

Comparing chemical environmental scores using USEtoxTM and CDV from the European Ecolabel

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Abstract

Purpose USEtoxTM (Rosenbaum et al. 2008) is a new model which can be used to calculate characterization factors for human and ecotoxicity impact categories used in life cycle assessment. The French ADEME-AFNOR (<http://affichage-environnemental.afnor.org/>) is currently considering this model to develop a new environmental labelling standard for consumer goods. The objective of this short study is to compare USEtoxTM impact scores with critical dilution volume (CDV) scores from the European Ecolabel (<http://ec.europa.eu/environment/ecolabel>), a well-established tool widely used in Europe aiming at discriminating environmental friendly products.

Material and methods The same range of chemicals (high scores to low scores) listed in both the USEtoxTM database and the EU Ecolabel detergent ingredient database (DID-list) were used for the comparison. The DID-list is a reference list, which contains agreed and verified fate and ecotoxicity data. The ranking was made based on two different ranking parameters, one from each model: the environmental impact score from USEtoxTM and the CDV from the EU Ecolabel. Additionally, a Spearman's rank correlation (ρ) coefficient was calculated.

Results and discussion Sixty-nine chemicals common in personal care and cleaning products were selected for

the comparison between USEtoxTM and EU Ecolabel methods. A “fair” agreement was found between the two models with a Spearman correlation coefficient ρ of 0.74, but a significant number of chemicals was ranked rather differently. The presence of outliers (i.e., different ranking) may be explained by several factors, which include the use of discrete versus continuous values to estimate the substance's degradation constant. Another factor could be that the substances are grouped under classes in the DID-list, thus having average parameter values. The main factor though probably lays in the different sources of the physico-chemical, fate and ecotoxicity data within the two model databases and the different way they are used for the ranking parameter calculation.

Conclusions Provided there is scientific consensus (and full transparency) on the raw data, both USEtoxTM and EU Ecolabel methods are relevant for ranking chemicals based on their physico-chemical and toxicological properties, and therefore for calculating product environmental impact scores related to their hazard. However, the presence of a number of chemicals with different ranking scores creates the risk of inconsistent consumer product information when either the CDV (EU ecolabel) or USEtoxTM (French “Affichage Environnemental”) is used for environmental labelling. To date, and for sake of consistency with an existing and used labelling scheme, the CDV appears much easier to implement with less uncertainty to calculate ecotoxicity impact score of products.

Keywords CDV · USEtoxTM · Chemical ranking · EU Ecolabel · Hazard for the environment · Product score

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1 Introduction

Since the year 2000, the life cycle assessment (LCA) community has started to develop new methods to characterise chemical impact on human and ecosystems using risk assessment (RA) concepts. The first methods to be developed were models such as USES-LCA (Huijbregts et al. 2000) and Impact 2002+ (Jolliet et al. 2003). Much of this work was initiated following the launch of the OMNIITOX program within the European framework FP6 program around the year 2002 (Molander et al. 2004). During the same period, the United Nations Environment Programme (UNEP) and the Society of Environmental Toxicology and Chemistry (SETAC) have launched the life cycle initiative and after several years of intense work and many workshops held with LCA and RA experts, the harmonised model USEtox™ was officially presented in SETAC in May 2010 (Rosenbaum et al. 2008). Although it is not the first life cycle impact assessment (LCIA) model, USEtox™ has received a lot of attention for two main reasons: (1) for the first time, a consensus has been reached on how to calculate chemical characterisation factors for the LCIA human and ecotoxicity impact categories; up to then the dozen of available models provided different results with variation up to nine orders of magnitude (Hauschild et al. 2008; Pant et al. 2004), obviously affecting the credibility of LCA; (2) these two impact categories were accepted by the international scientific community and/or approved by the competent international organisations UNEP and SETAC, thus complying with one of the ISO standard requirements (see ISO 14044).

USEtox™ is probably one of the most reliable chemical ranking tools, provided that all the data needed to run the model are available and of good quality. However, other tools could be used to rank chemicals, like the critical dilution volume (CDV) scores used in the EU Ecolabel scheme, a well-established tool widely used in Europe to identify environmental friendly products. EU Ecolabel is a multicriteria system with CDV being one criterion for freshwater toxicity impact assessment. The objective of this paper is to compare the pertinence of the USEtox™ model with the CDV model, both used to discriminate environmentally friendly product, to rank chemicals (and products) in the context of the French environmental product labelling.

2 Methods

The 69 chemicals listed in both the USEtox™ database and the EU Ecolabel detergent ingredient database (DID-list) and for which the USEtox™ database has data for the 15 parameters needed, were used for the comparison. The DID-list is a reference list which contains agreed and verified fate and ecotoxicity data. The ranking was made

based on two different ranking parameters, one from each model: the environmental impact score (IS) (USEtox™) (Rosenbaum et al. 2008) and the CDV (EU Ecolabel) (<http://ec.europa.eu/environment/ecolabel>).

In USEtox™, the hazard associated with a substance i is represented by its ecotoxicity characterization factor (CF_i) which represents the substance potency for the specific category of impact, in this case ecotoxicity, and is independent from the substance quantity. The CF_i [potentially affected fraction (PAF) per cubic metre per kilogram per day] includes information about the chemical toxicity [ecological effect factor (EF)], about its fate in the environment (fate factor and exposure factor) (Rosenbaum et al. 2008). The IS for ecotoxicity is the sum of the CF_i of each compartment (urban air, rural air, freshwater and agricultural soil) multiplied by the weight of the ingredient, set here to unity for comparison purposes (Rosenbaum et al. 2008). The CF factors associated with compartment-specific emission are listed in the USEtox™ database of organic chemicals.

In the EU Ecolabel model, the hazard associated with a substance i is represented by its CDV. The CDV (in litres per gram) is the volume of water necessary to dilute a chemical to a safe concentration and is calculated as follows:

$$CDV(\text{substance } i) = w(i) \times DF(i) \times 1,000/TF(i)$$

where $w(i)$ is the weight of the ingredient (in grams) per functional unit (i.e., grams of active compounds) set to 1 for comparison purposes, $DF(i)$ is the degradation factor and $TF(i)$ is the toxicity factor of the ingredient (in milligrams per litre). DF is directly related to biodegradability and $TF(i)$ is the lowest ecotoxicity data divided by an assessment factor ranging from 10,000 to 10 depending on the number and the type of data available, (<http://ec.europa.eu/environment/ecolabel>). $TF(i)$ and $DF(i)$ are derived by the EU commission and industry representatives for about 200 chemicals used in personal care and cleaning products on the classical risk assessment approach [technical guidance document (TGD); (Van Leeuwen 2003)]. The CDV is calculated using the data from the official DID-list part A for soap and shampoo downloaded from the EU Ecolabel website (<http://ec.europa.eu/environment/ecolabel>). Due to the grouping system in the DID-list, several chemicals can have the same CDV score but different IS scores. In the case several chemicals have the same CDV ranking score, an average score is attributed to them (Table 1).

To test the correlation between the CDV ranking score (x_i) and the IS ranking score (y_i), a Spearman rank correlation coefficient (ρ) was calculated, as follows:

$$\rho = \frac{6 \sum di^2}{n(n^2 - 1)}$$

Table 1 Ranking scores using the CDV of the EU Ecolabel model and the USEtox™ model and comparison factor γ for the 69 chemicals compared

Chemical names	EU Ecolabel ranking score	USEtox™ ranking score	Comparison factor γ
2-Methyl-2H-isothiazol-3-one (MIT)	1	1	0.000
Triclosan	2	2	0.000
CMI + MIT in mixture 3:1	3	3	0.000
Lauryl trimethyl ammonium chloride (C12)	4.5	4	0.007
Cetyltrimethylammonium chloride (C16)	4.5	5	−0.007
Methyldibromo glutaronitrile	6	8	−0.029
2-Bromo-2-nitropropane-1,3-diol	7	11	−0.058
Glutaraldehyde	8	12	−0.058
1-Decanol	9.0	16	−0.101
Dodecanoic acid	10.0	24	−0.203
o-Phenylphenol	11.0	9	0.029
Sodium dioctyl sulfosuccinate	12.5	23	−0.152
Sodium dioctyl sulfosuccinate	12.5	27	−0.210
Trimethyl pentanediol monoisobutyrate	14.0	25	−0.159
Formaldehyde	15.0	22	−0.101
Sulphamic acid	16.0	17	−0.014
FWA 5	17.0	62	−0.652
Polyethylene glycol ethers of C12-C14 alcohols, C12-14EO7	19.5	19	0.007
Monoethanolamine	19.5	31	−0.167
Diethanolamine	19.5	38	−0.268
Triethanolamine	19.5	46	−0.384
Sodium lauryl ether sulphate	23.0	7	0.232
Ethanol, 2-[2-[2-(dodecyloxy)ethoxy]ethoxy]-, hydrogen sulphate, sodium salt	23.0	14	0.130
Urea	23.0	47	−0.348
Salicylic acid	25.0	30	−0.072
Malonic acid	26.0	33	−0.101
HEDP, phosphonates	28.5	18	0.152
ATMP, phosphonates	28.5	21	0.109
DTMP, phosphonates	28.5	36	−0.109
DTPMP Na5, phosphonates	28.5	45	−0.239
Oxalic acid	31.0	44	−0.188
1-Hexadecanol, hydrogen sulphate, sodium salt	34.5	6	0.426
1-Tetradecanol, hydrogen sulphate, sodium salt	34.5	10	0.368
Sulfuric acid, monododecyl ester sodium salt	34.5	15	0.296
Sulfuric acid, monododecyl ester, ammonium salts	34.5	20	0.223
Sodium decyl sulphate	34.5	35	0.006
Sodium octyl sulphate	34.5	54	−0.270
Acetic acid	34.5	34	0.058
EDTA Na4	34.5	39	0.007
EDTA	34.5	40	−0.007
Clay (insoluble inorganic), e.g., Bentonite, Montmorillonite	41.0	63	−0.319
Benzenedodecylsulfonic acid, sodium salt	42.0	13	0.420
Formic acid (Ca salt)	43.5	37	0.094
Formate-Na	43.5	57	−0.196
Maleic acid	45.0	28	0.246
Sodium benzoate	46.0	29	0.246
L + -lactic acid	47.0	41	0.087

Table 1 (continued)

Chemical names	EU Ecolabel ranking score	USEtox™ ranking score	Comparison factor γ
Ethylene glycol monobutyl ether/2-Butoxyethanol	48.0	50	−0.029
Diethylene glycol monomethyl ether	49.0	49	0.000
Benzyl alcohol	50.0	26	0.348
Diethylene glycol	51.5	67	−0.225
Triethylene glycol	51.5	68	−0.239
1-Methyl-2-pyrrolidone	53.0	48	0.072
Diethylene glycol monoethyl ether	54.0	65	−0.159
Glycerol	55.0	69	−0.203
Butan-2-ol	58.5	51	0.109
Butan-1-ol	58.5	52	0.094
Ethanol	58.5	56	0.036
Propan-1-ol	58.5	58	0.007
Methanol	58.5	60	−0.022
Propan-2-ol	58.5	61	−0.036
Diethylene glycol monobutyl ether	62.0	55	0.101
Nitrilotriacetic acid	63.5	32	0.457
Nitrilotriacetic acid, Na3	63.5	42	0.312
Citric acid	65.5	43	0.326
Citric acid, Na3 salt	65.5	59	0.094
1-Methoxypropan-2-ol	67.0	53	0.203
Ethylene glycol/ethane-1,2- diol	68.0	64	0.058
Propylene glycol/propane-1,2-diol	69.0	66	0.043

The five chemicals with the largest discrepancies in their ranking score are highlighted in bold

with $d_i = x_i - y_i$. The Spearman correlation coefficient is a non-parametric measure of statistical dependence between two ranked variables. A ρ of 1 would reflect a perfect correlation between the two variables, whereas a ρ of 0 would reflect no correlation at all.

In order to identify outliers, a factor γ was calculated using the following equation:

$$\gamma = \frac{x_i - y_i}{69}$$

Where γ can range from −1 to +1. The outliers are characterised by large absolute values of γ (i.e., $|\gamma|$), as these represent larger discrepancies between model results. A $|\gamma| \rightarrow 0$ indicates a mutual agreement between the two model predictions. Moreover, a negative γ indicates that the CDV prediction is more alarmist, and inversely, a positive γ indicates that the IS prediction is more alarmist.

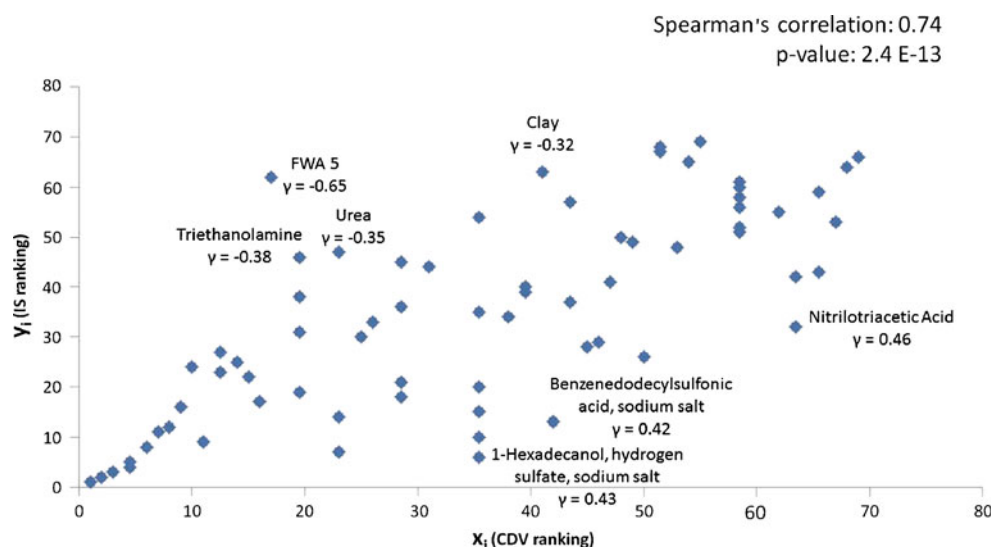
3 Results and discussion

The calculated Spearman correlation coefficient is 0.74, which is considered an overall “fair” correlation between the Ecolabel CDV model and the Usetox™ model, as shown in Fig. 1. A p value of 2.4E-13 confirms the validity of the

statistical result. However, a significant number of outliers can be observed suggesting some disagreements between the two models. The ranking score using the CDV model and the USEtox™ model as well as the corresponding comparison factor γ are shown in Table 1. The first observation is that both USEtox™ and the CDV model identified the same five most hazardous chemicals and rank them in the same order. Furthermore, among the 69 substances studied, five are classified in the annex I of the Dangerous Substances Directive (67/548/EEC) as toxic for the environment (R50, R51, R52 and R53). Those five substances have been classified by both USEtox™ and CDV between the second and the 17th position of the ranking, i.e., among the predicted first quarter of most hazardous chemicals of our list.

The differences between the two ranking systems might be explained by several factors. First of all, it is important to point out that the CDV model uses only two parameters (DF and TF), whereas the USEtox™ model uses a minimum of eight parameters for the calculation of the fate factor, six parameters for the exposure factor, and another single parameter (HC50) for the effect factor, which makes a total of 15 parameters needed to estimate CF and therefore the IS. As the relative error associated with the IS or CDV is the sum of the relative error associated with each of the

Fig. 1 Relation between the ranking scores of chemicals calculated with the Ecolabel CDV (x_i) and the UsetoxTM IS (y_i)



parameters used to calculate them, it is likely that the error associated with the IS is larger than the error associated with the CDV. Even though the information about the error associated with each of those parameters is not available, the precision of the IS is, according to Rosenbaum et al. (2008), within a factor 10–100 for freshwater ecotoxicity.

It is interesting to note that UsetoxTM is not designed in particular to deal with organic materials nor with substances with dissociating chemistries or surface active compounds, whereas any chemical can be assessed with CDV. If the only inorganic chemical is removed from the list, as well as salts, the Spearman rank correlation coefficient increases to 0.79.

The differences might also be explained by the different sources of ecotoxicity and degradation data between the two models. CDV uses four discrete degradation factors ranging from 0.05 to 1 for readily biodegradable and persistent substances, respectively. According to the 2003 EU TGD (Van Leeuwen 2003), these established degradation categories correspond to rate constant (k) and half-lives, as reported in Table 2. USEtoxTM IS is calculated based on degradation rate constants, not categorised, but on a continuous scale. Moreover, USEtoxTM degradation factor includes, in theory, all degradation processes, i.e., photo-degradation and abiotic degradation, whereas the CDV degradation factor reflects only biodegradation. However, many experimental degradation constants are lacking in the USEtoxTM database and in the absence of experimental data, USEtoxTM estimates the degradation constants using EPI-WIN software which computes only biodegradation rates for the freshwater compartment (Table 3). Therefore, the half-lives extrapolated for USEtoxTM and the CDV are comparable for most substances, as shown in Table 2. It is reasonable to think that the lack of data in the USEtoxTM database will be overcome as soon as experimental data will become available (i.e., via REACH, EC 1907/2006).

The most obvious difference in degradation data can be observed for nitrotriacetic acid (NTA) which has a half-life of 150 days according to the CDV model and a half-life of 9 days according to the USEtoxTM. Although this latter model foresees a faster decrease of NTA concentration in the environment, the chemical ranks 32 by USEtoxTM and 63.5 by CDV, thus being considered of higher concern by USEtoxTM. The large discrepancy in the ranking scores by the two models for NTA is reflected by the large γ value of 0.457.

This discrepancy cannot be explained by differences in the ecotoxicity data either. TF (CDV) is 1.28 mg/L and average HC50 (USEtoxTM) is 70.8 mg/L, and in both models, the ranking is inversely proportional to this value. The remaining parameter which could decrease USEtoxTM IS value is the exposure factor which estimates the chemical fraction in the selected compartment, i.e., freshwater and which is always lower than 1. Since this parameter is not present in the CDV method, a direct comparison is not possible. At this stage, it is not possible to definitively identify if the DID-list is underestimating NTA hazard or if USEtoxTM overestimates it. The ranking of nitrotriacetic acid trisodium salt in position 42 of USEtoxTM may indicate that NTA ranking is overestimated in USEtoxTM: these two compounds are linked through acid–base equilibria and therefore their ranking scores should be the same because they can interconvert as a function of the local pH.

In USEtoxTM, the toxicity factor, which is called the ecotoxicological EF is derived from the average of the chronic EC50, over all species (HC50), whereas the CDV TF is based on the ecotoxicity test results for the most sensitive species divided by a safety factor ranging from 10,000 to 10, depending on the type of data (acute/chronic) and the number of trophic levels represented. Therefore, we

Table 2 Comparison of the degradation data used in the two models studied for the five chemicals with highest $|\gamma|$ and two chemicals with the lowest $|\gamma|$

Chemicals with highest $ \gamma $	EU Ecolabelling		USEtox™			
	DF DID-list	Half-life (days) ^a	k (d ⁻¹) ^a	$k_{\text{deg., water}}$ (s ⁻¹)	$k_{\text{deg., water}}$ (d ⁻¹)	Assigned half-life (days) ^b
FWA-5 (27344-41-8)	1	8	0	2.110^{-7c}	1.910^{-2}	37.5
1-Hexadecanol, hydrogen sulphate, sodium salt (1120-01-0)	0.05	15	4.710^{-2}	5.410^{-7c}	4.610^{-2}	15
Benzenedodecylsulfonic acid, sodium salt (25155-30-0)	0.05	15	4.710^{-2}	5.410^{-7c}	4.610^{-2}	15
Nitrilotriacetat (NTA) (139-13-9)	0.5	150	4.710^{-3}	9.310^{-7c}	8.010^{-2}	8.7
Triethanolamine (102-71-6)	0.05	15	4.710^{-2}	5.410^{-7c}	4.610^{-2}	15
Chemicals with lowest $ \gamma $						
2-Methyl-2H-isothiazol-3-one (MIT) (2682-20-4)	0.5	150	4.710^{-3}	5.410^{-7c}	4.610^{-2}	15
Triclosan (3380-34-5)	0.5	150	4.710^{-3}	1.310^{-7c}	1.110^{-2}	60

DF degradation factor, DID-list detergent ingredient database

^a The half-life values and the degradation constant k as defined in the TGD for risk assessment, part II

^b Assigned half-life as described in the “USEtox™ chemical database: organics manual”

^c Estimated (EPIWIN) values from the USEtox™ database

would expect the ranking of the CDV to be on average more alarmist than USEtox™ ranking, but this is not observed in our ranking comparison. The USEtox™ ecotoxicity values come either from the Payet database (Payet 2004) or are derived from RIVM e-toxBase database (<http://e-toxbase.com>) or from Ecotox database (<http://cfpub.epa.gov/ecotox/>); when chronic EC50 values are missing, USEtox™ converts acute data with appropriate conversion factors. It is therefore difficult to compare the ecotoxicity data used in both models, but the data in Table 3 show that the discrepancies in the ecotoxicity data alone cannot explain the difference in the ranking score.

In USEtox™, individual physico-chemical, fate and ecotoxicity data are attributed to each substance, whereas in the Ecolabel DID-list, substances with similar chemical formulae are grouped and only one ecotoxicity data value is attributed per group. In some cases, two substances which are part of the same head group in the DID-list are attributed very different ecotoxicity values in USEtox™. The most striking examples are sodium “octyl sulphate” and “1-Hexadecanol hydrogen sulphate sodium salt”; both grouped in the DID-list under the head title “C8/10 Alkyl sulphate” to which an LC50/EC50 of 132 mg/L is attributed. In the USEtox™ database though, “octyl sulphate” and “1-Hexadecanol hydrogen sulphate sodium salt” have an average EC50 (HC50) of 3,981 and 0.33 mg/L, respectively.

Less dramatic, but nevertheless perturbing, are the differences in ecotoxicity values assigned in USEtox™ to chemicals which differ only by their acid–base equilibrium (e.g., NTA and NTA trisodium salt) or by their counter ions.

Sodium formate for example, has an EC50 of 29.9 mg/L, while calcium formate has an EC50 of 8.2 mg/L. This seems to confirm that USEtox™ is not particularly designed to deal with acid–base equilibria. A critical review of the source data of both USEtox™ and DID-list are necessary to understand the source of these differences. Although this work is beyond the scope of this publication, it is chemically more reasonable to assign the same ecotoxicity value to an acid–base couple.

It should also be considered that CDV evaluates only the freshwater compartment and at the best of our knowledge, the hazard assessment in other compartments (e.g., sediment, soil, air) will not be implemented in the future. On the contrary, USEtox™ is developed to evaluate the hazard in five compartments both at continental and global scale and fluxes of substances among these compartments. However, in our comparison, the USEtox™ ranking was not greatly changed, if only the CF for the freshwater compartment was accounted for in the IS calculation or if the sum of the CF for all compartments (urban air, rural air, freshwater and agricultural soil) was used to calculate the ecotoxicity IS (data not shown). As mentioned above, USEtox™ is designed to deal in particular with organic materials, whereas a CDV can be calculated for any chemical. Last but not least, a major difference regarding the purpose and the use of both models has to be noticed: Ecolabel is the result of strict environmental (pass/fail) criteria agreed at the EU level to encourage business to market products and services that are friendly to the environment, i.e., with less hazardous chemicals. The CDV is easy to use and to calculate and requires fewer

Table 3 Comparison of the ecotoxicity data used in the EU Ecolabel (EC_{50}/LC_{50} of the DID-list, based on more sensitive species) and the USEtoxTM models [average of the chronic EC_{50} , over all species (HC_{50})] for the five chemicals with highest $|\gamma|$ and two chemicals with the lowest $|\gamma|$

Chemicals with highest $ \gamma $	EU Ecolabelling				USEtox TM			
	EC50/LC50		NOEC		Safety factor		TF	
	DID-list (acute)		DID-list (chronic)		DID-list		DID-list	
							USEtox TM database	
FWA-5 (27344-41-8)	10		1		10		1.09	12.3
1-Hexadecanol, hydrogen sulphate, sodium salt (1120-01-0)	132		–		5000		–0.48	0.33
Benzenedodecylsulfonic acid, sodium salt (25155-30-0)	4.1		0.69		10		0.49	3.09
Nitritriacetat (NTA) (139-13-9)	494		64		50		1.85	70.8
Triethanolamine (102-71-6)	90		0.78		100		2.82	660
Chemicals with lowest $ \gamma $								
2-Methyl-2H-isothiazol-3-one (MIT) (2682-20-4)	0.06		–		1000		–1.29	0.05
Triclosan (3380-34-5)	0.0014		0.00069		10		–0.75	0.18

DID-list detergent ingredient database, *NOEC* no observed effect concentration

data. On the contrary, USEtoxTM is an LCA tool, designed to estimate global impact of a product over its entire life cycle, but is rather complicated to understand and to use, and requires a lot of data that are often lacking. Of course, thanks to REACH, the data gap should decrease with time, but it remains a big issue for the time being.

In our view, there is an emerging concern about the misuse of USEtoxTM within the non-specialists. Since USEtoxTM is an LCA model which integrates (merges) many methodological aspects of risk assessment, the temptation to think that one tool can do all is rather high among non-risk assessment specialists.

4 Conclusions

The comparison between the CDV ranking scores from the EU Ecolabel and USEtoxTM has demonstrated that both models identify the same five chemicals of highest concern for the environment and that there is an overall “fair” agreement between the two models. However, the differences between the two model ranking scores cannot solely be explained by the differences in the degradation or ecotoxicity data; a case by case study may be necessary to understand the reason for different ranking scores. To do so, it is of great importance to understand how raw data used in both systems were selected, therefore full transparency is needed.

Within the AEDEME/AFNOR French product environmental information standard development, one could challenge the pertinence of using USEtoxTM over the CDV. It is very important that both systems provide the same recommendation to consumers regarding a product’s environmental impact. Therefore, before choosing any model, it is important to understand why in some cases the two systems provide different ranking results. In the end, whatever method is selected, one will need to demonstrate that the environment will truly benefit from it.

Furthermore, to date, USEtoxTM seems more cumbersome to implement. Why go for a complicated scheme when a simple one provides a similar answer? In a more distant future, with the acquisition and validation of the necessary data to evaluate the 15 parameters necessary to calculate the IS and if the difficulty around the assessment of dissociating chemicals is resolved, the USEtoxTM model might be used for chemical ranking based not only on their freshwater ecotoxicity but also for other environmental compartments.

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